PARTIAL WAVES IN THREE DIMENSIONS - HARD SPHERE SCATTERING

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In our earlier look at partial wave analysis in quantum scattering, we found that for scattering of an incident plane wave from a spherically symmetric potential, the overall wave function for the region outside the influence of the potential is

$$\psi(r,\theta)=A\sum_{l=0}^{\infty}i^{l}(2l+1)\left[j_{l}(kr)+ika_{l}h_{l}^{(1)}(kr)\right]P_{l}(\cos\theta) \tag{1}$$

where $k=\sqrt{2mE}/\hbar$, j_l is a spherical Bessel function, $h_l^{(1)}$ is a Hankel function of the first kind and P_l is a Legendre polynomial. The partial wave coefficients a_l must be determined by solving the Schrödinger equation for the scattering region (where $V\ne 0$) and matching that solution to the above wave function using boundary conditions.

It turns out that there is another way of writing the wave function in the outer region, using phase shifts. For a spherically symmetric potential $V(r)$, the force is the negative gradient of the potential, and is always parallel to $\hat{\mathbf{r}}$. This means that the torque $\mathbf{N}=\mathbf{r}\times\mathbf{F}=0$ for such a potential, so total angular momentum is conserved: $\dot{\mathbf{L}}=I\mathbf{N}=0$, where I is the moment of inertia. This means that the amplitude of the lth component of the incident wave must be equal to the amplitude of the lth component of the scattered wave in 1, although the scattering may introduce a phase shift, just as in the one-dimensional case.

Griffiths goes through the details of the derivation of the phase shift in his section 11.3. The basic idea is to write the wave function for the incoming plane wave on its own (when $V=0$ so there is no scattering):

$$\psi_0=A\sum_{l=0}^{\infty}i^{l}(2l+1)j_{l}(kr)P_{l}(\cos\theta) \tag{2}$$

and then take its asymptotic form as $kr\gg 1$:

$$\psi_0\approx\frac{A}{2ikr}\sum_{l=0}^{\infty}i^{l}(2l+1)\left(e^{ikr}-(-1)^{l}e^{-ikr}\right)P_{l}(\cos\theta) \tag{3}$$

We now write a wave function for the case where there *is* some scattering, so that $V\neq0$, by introducing a phase shift $2\delta_l$ in the outgoing wave term for each partial wave:

$$\psi\approx\frac{A}{2ikr}\sum_{l=0}^{\infty}i^l\left(2l+1\right)\left(e^{i(kr+2\delta_l)}-(-1)^l e^{-ikr}\right)P_l\left(\cos\theta\right) \tag{4}$$

Each term in the sum is one partial wave with angular momentum number l, and we know that the amplitudes of each incoming and scattered partial wave for each individual value of l must be the same, due to conservation of angular momentum.

Of course, we still need to find the phase shifts δ_l and to do that, we need to solve the Schrödinger equation in the region where $V\neq0$ and match it to 4 using boundary conditions, so there isn't really any saving in the amount of work we need to do to find the scattering amplitudes. However, the phase shift is real, while the a_ls in 1 are often complex, and phase shifts have a physical interpretation that is easier to understand than the abstract a_l coefficients.

To derive the relation between δ_l and a_l, we compare the asymptotic form of 1 with 4 (details in Griffiths), and we find that

$$a_l=\frac{e^{2i\delta_l}-1}{2ik}=\frac{1}{k}e^{i\delta_l}\sin\delta_l \tag{5}$$

We can invert this to get

$$\delta_l=\frac{1}{2i}\ln\left(2ika_l+1\right) \tag{6}$$

The overall scattering amplitude and cross section are

$$f\left(\theta\right)=\frac{1}{k}\sum_{l=0}^{\infty}\left(2l+1\right)e^{i\delta_l}\sin\delta_l P_l\left(\cos\theta\right) \tag{7}$$

$$\sigma=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}\left(2l+1\right)\sin^2\delta_l \tag{8}$$

Example 1. Hard sphere scattering phase shifts. We've already found the a_ls for the hard sphere case:

$$a_l=i\frac{j_l\left(ka\right)}{kh_l^{(1)}\left(ka\right)} \tag{9}$$

Using 6 to find δ_l is a bit tricky, since the complex logarithm is multi-valued. It's easier to work from 5. From the definition of $h_l^{(1)}$ we have

$$h_l^{(1)} \equiv j_l + i n_l \tag{10}$$

$$a_l = i \frac{j_l}{k\left(j_l + i n_l\right)} \tag{11}$$

$$= \frac{i}{k} \frac{j_l\left(j_l - i n_l\right)}{j_l^2 + n_l^2} \tag{12}$$

$$= \frac{j_l}{k\left(j_l^2 + n_l^2\right)}\left(n_l + i j_l\right) \tag{13}$$

We can write this in modulus-argument form:

$$|a_l| = \frac{|j_l|\sqrt{j_l^2 + n_l^2}}{k\left(j_l^2 + n_l^2\right)} \tag{14}$$

$$= \frac{|j_l|}{k\sqrt{j_l^2 + n_l^2}} \tag{15}$$

$$\delta_l = \arg a_l = \arctan \frac{j_l}{n_l} \tag{16}$$

When comparing this with 5 we have to be careful to get the right quadrant for δ_l. We do this in the usual way by looking at the signs of j_l and n_l. If they are both positive, then δ_l is in the first quadrant, if $j_l > 0$ and $n_l < 0$, we're in the second quadrant, and so on.

PINGBACKS

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